B2 cancl

9. (Amended) The computer system of claim 1, wherein the chemical compounds include compounds obtained from natural sources that exhibit biological activity.

B3

27. (New) The computer system of claim 1, wherein the interaction includes binding.

28. (New) The computer system of claim 1, wherein the chemical compounds include compounds with known biological activity or that have failed in preclinical or human clinical tests.

29. (New) The computer system of claim 1, wherein the chemical compounds include compounds used in commerce as herbicides or pesticides.

30. (New) The computer system of claim 1, wherein the chemical compounds include known pharmaceuticals approved for human clinical use by the Food and Drug Administration.

31. (New) The computer system of claim 1, wherein the molecular targets include ion channels.

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

32. (New) The computer system of claim 1, wherein the molecular targets include transporters or uptake sites.

33. (New) A computer system comprising:

a first datastore containing data corresponding to a plurality of chemical compounds;

a second datastore containing data corresponding to a plurality of molecular targets;

a third datastore containing data corresponding to tests of interactions between compounds in the first datastore and molecular targets in the second datastore; and

a user interface allowing a user to view information from the first datastore, the second datastore, and the third datastore as it relates to a compound record in the first datastore or as it relates to a molecular target in the second datastore or as it relates to one or more interaction records in the third datastore.

34. (New) The computer system of claim 33, wherein the chemical compounds include compounds with known biological activity.

B3

35. (New) A computer system comprising:

a first database containing data corresponding to a plurality of chemical compounds and data corresponding to biological information related to effects of such chemical compounds on biological systems;

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

a second database containing data corresponding to a plurality of molecular targets;

a third database containing data corresponding to tests of interactions between compounds in the first database and molecular targets in the second database; and

a user interface allowing a user to view data from the first database, the second database, and the third database as it relates to at least one compound in the first database or as it relates to at least one molecular target in the second database or as it relates to one or more interactions in the third database.

36. (New) The computer system of claim 35, wherein the chemical compounds include compounds with known biological activity.

37. (New) A computer system comprising:

a first database containing records corresponding to a plurality of chemical compounds and records corresponding to biological information related to effects of such chemical compounds on biological systems;

a second database containing records corresponding to a plurality of molecular targets; and

a third database containing records corresponding to tests of interactions between compounds in the first database and molecular targets in the second database, the tests including information on the effect that a compound from the plurality of compounds has on the interaction of a compound known to interact with a molecular target from the plurality of molecular targets and said molecular target.

B3

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

38. (New) The computer system of claim 37, further comprising:

a user interface allowing a user to view information from at least one of the first database, the second database, and the third database as it relates to a compound record in the first database.

39. (New) The computer system of claim 37, further comprising:

a user interface allowing a user to view information from at least one of the first database, the second database, and the third database as it relates to a molecular target in the second database.

40. (New) The computer system of claim 37, further comprising:

a user interface allowing a user to view information from at least one of the first database, the second database, and the third database as it relates to one or more interaction records in the third database.

41. (New) The computer system of claim 37, wherein the interaction includes binding.

42. (New) The computer system of claim 37, wherein the interaction includes binding and the effect includes inhibitory effect.

B3

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

43. (New) The computer system of claim 37, wherein the chemical compounds include compounds with known biological activity.

44. (New) A memory for storing data for access by a process being executed by a processor, the memory comprising:

a data structure for maintaining (i) a first set of information associated with one or more chemical compounds, (ii) a second set of information associated with one or more molecular targets, and (iii) a third set of information reflecting an interaction between the chemical compounds and the molecular targets, wherein the process may provide, based on one or more queries, information reflecting a relationship between a chemical compound included in the first set, a molecular target included in the second set, and the information included in the third set.

45. (New) In a system for correlating data associated with chemical compounds and molecular targets, a memory comprising:

a first array of records, each including information indicative of a chemical compound;

a second array of records, each including information indicative of a molecular target;

a third array of records, each corresponding to a binding capability between each of the chemical compounds and molecular targets; and

a fourth array of records, each corresponding to a biological activity related to the chemical compounds and the molecular targets,

B3

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

wherein a process may access the first, second, and third arrays to produce information corresponding to a drug potential for a new compound based on relationships between characteristics associated with the new compound and a selected biological activity included in the fourth array of records or patterns of binding capabilities included in the third array.

46. (New) A memory device for storing data for access by a process executed by a processor, the memory device comprising:

a compound data structure including data associated with a set of chemical compounds;

a target data structure including data associated with a set of molecular targets; and

a result data structure including data corresponding to results of screening tests between chemical compounds and molecular targets,

wherein the process determines a relationship between the data included in the compound, target, and result data structures.

47. (New) The memory device of claim 46, wherein the results include information on an effect a selected compound has on a known interaction of another compound with a selected molecular target and an effect of the selected compound with the selected molecular target.

B3

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

48. (New) The memory device of claim 46, wherein the chemical compounds include at least one of:

(i) compounds with known biological activity,

(ii) compounds tested in animals,

(iii) compounds known to have an effect on the environment,

(iv) pharmacological reference agents,

(v) known pharmaceuticals that have available preexisting biological information,

(vi) compounds approved by a government agency for testing in humans, and

(vii) compounds obtained from natural sources that exhibit biological activity.

49. (New) The memory device of claim 46, wherein the molecular targets include at least one of:

(i) receptors,

(ii) enzymes,

(iii) nucleic acids,

(iv) carbohydrates,

(v) ion channels, and

(vi) transporters or uptake sites.

B3

50. (New) The memory device of claim 46, wherein the process also provides a graphical interface including a description and properties of a selected chemical compound included in the compound data structure.

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

51. (New) The memory device of claim 50, wherein the graphical interface includes a representation of at least one of the selected compound's name, type, structure, physical-chemical characteristics, chemical structural descriptors, and solubility.

52. (New) The memory device of claim 46, including a biological data structure including information corresponding to biological information related to an effect of each chemical compound included in the compound data structure on each molecular target included in the target data structure.

53. (New) The memory device of claim 52, wherein the biological information includes at least one of side effects, toxicity, and mechanism of drug action.

54. (New) In a system for maintaining test screening results, a storage device for storing data for access by a processor comprising:

a data set including information corresponding to results of tests that show an interaction between selected chemical compounds and selected molecular targets,

wherein the process provides selected result information to another data set based on a request associated with a selected chemical compound or molecular target.

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

55. (New) The system of claim 54, wherein the results are represented in a form that reflects whether each chemical compound binds with a corresponding molecular target.

56. (New) The system of claim 54, wherein the results are represented in a form that reflects a potency of a binding between each chemical compound and a corresponding molecular target.

57. (New) A computer-readable medium for storing information associated with molecular targets, comprising:

a first data array including information reflecting a relationship between identifiers and types of molecular targets;

a second data array including information reflecting characteristics of a first type of molecular target included in the first data array; and

a third data array including information reflecting characteristics of a second type of molecular target included in the first data array,

wherein a program, when executed by a processor, retrieves information from either the second or third data array based on a request for a selected molecular target, or a request for a selected type of molecular target, included in the first data array.

B3

58. (New) A system comprising:

a memory including one or more data arrays of information associated with chemical compounds and molecular targets; and

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

a processor for executing a process for providing a user interface including:

a representation of a selected chemical compound,

description information associated with the selected chemical compound, and

biological information associated with the selected chemical compound.

59. (New) A computer system comprising:

a first database containing records corresponding to a plurality of known biologically active chemical compounds,

a second database containing records corresponding to a plurality of molecular targets;

a third database containing records corresponding to the results of tests to determine the interaction between compounds in the first database and targets in the second database; and

a user interface allowing a user to view data from the first database, the second database, and the third database as it relates to at least one compound in the first database or as it relates to at least one molecular target in the second database or as it relates to one or more interactions in the third database.

60. (New) The computer system of claim 59, wherein the third database includes records corresponding to the results of tests to determine the interaction between all or substantially all of the compounds selected to comprise a compound set in the first database and all or substantially all of the molecular targets selected to comprise a molecular target set in the second database.

B3

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

61. (New) The computer system of claim 59, wherein the third database includes records corresponding to the results of tests to determine the interaction between a majority of the compounds selected to comprise a compound set in the first database and a majority of the molecular targets selected to comprise a molecular target set in the second database.

62. (New) The computer system of claim 59, further comprising:

a fourth database containing records corresponding to the effect of chemical compounds contained in the first database on biological systems

63. (New) The computer system of claim 62, wherein the third database includes records corresponding to the results of tests to determine the interaction between all or substantially all of the compounds selected to comprise a compound set in the first database and all or substantially all of the molecular targets selected to comprise a molecular target set in the second database.

64. (New) The computer system of claim 62, wherein the third database includes records corresponding to the results of tests to determine the interaction between a majority of the compounds selected to comprise a compound set in the first database and a majority of the molecular targets selected to comprise a molecular target set in the second database.

B3

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

65. (New) The computer system of claim 59, wherein the first database contains records corresponding to a plurality of known biologically active chemical compounds selected from among representatives of the following categories:

(a) pharmacological reference agents used in receptor, ion channel, transporter, or enzyme screening assays;

(b) drug candidates that have been approved by the Food and Drug Administration for testing in humans, including those that have been discontinued from further development; and

(c) pharmaceuticals that have been approved for human clinical use by the Food and Drug Administration, including those that have been subsequently withdrawn from the market.

66. (New) The computer system of claim 65, wherein the known biologically active compounds included in the first database are further selected from among the following:

compounds that have been tested in preclinical studies in animals;

pesticides;

herbicides;

bioactive natural products;

agricultural chemicals; and

environmental chemicals.

B3

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

67. (New) The computer system of claim 59, wherein the second database contains records corresponding to a plurality of molecular targets selected from among representatives of the following categories:

(a) receptors;

(b) ion channels;

(c) transporters or uptake sites; and

(d) enzymes.

68. (New) The computer system of claim 65, wherein the second database contains records corresponding to a plurality of molecular targets selected from among representatives of the following categories:

(a) receptors;

(b) ion channels;

(c) transporters or uptake sites; and

(d) enzymes.

69. (New) The computer system of claim 67, wherein the molecular targets in the second database are related to drug discovery and development.

B3

70. (New) The computer system of claim 59, wherein the third database contains records corresponding to statistically complete results of tests to determine the interaction between compounds in the first database and targets in the second database.

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

71. (New) The computer system of claim 59, wherein the records in the third database corresponding to the results of tests to determine the interaction between compounds in the first database and targets in the second database includes positive interactions and negative or lack of interactions.

72. (New) The computer system of claim 59, wherein the tests to determine the interaction between compounds in the first database and the targets in the second database are based on binding interactions.

73. (New) The computer system of claim 59, wherein the tests to determine the interaction between compounds in the first database and the targets in the second database measure the inhibition of binding by a compound in the first database with respect to a target in the second database in the presence of another compound, such as a reference agent or enzyme substrate, known to interact with the target.

74. (New) The computer system of claim 59, wherein the tests used to generate results comprising the third database are ligand binding assays.

B3

75. (New) The computer system of claim 59, wherein the tests used to generate results comprising the third database are enzyme inhibition assays.

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

76. (New) The computer system of claim 59, wherein the tests to determine the interaction between compounds in the first database and the targets in the second database measure functional activation, functional enhancement, functional inhibition, or lack of functional effect with respect to the molecular target.

77. (New) The computer system of claim 59, wherein the tests used to generate results comprising the third database measure adenyl cyclase activity, inositol triphosphate, or neurotransmitter transport.

78. (New) The computer system of claim 59, wherein the tests used to generate results comprising the third database are based on reporter gene assays or cellular functional assays.

79. (New) The computer system of claim 59, wherein the results of tests to determine the interaction between compounds in the first database and targets in the second database are recorded in the third database as numerical values.

80. (New) The computer system of claim 59, wherein the results of tests to determine the interaction between compounds in the first database and targets in the second database are recorded in the third database as per cent inhibition values.

B3

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

81. (New) The computer system of claim 59, wherein the results of tests to determine the interaction between compounds in the first database and targets in the second database are recorded in the third database as potency values.

82. (New) The computer system of claim 59, wherein the results of tests to determine the interaction between compounds in the first database and targets in the second database are organized in the third database in terms of whether or not the interaction values exceed a specified threshold.

83. (New) The computer system of claim 59, wherein the results of tests to determine the interaction between compounds in the first database and targets in the second database are organized in the third database in terms of whether or not the interaction values fall below a specified threshold.

84. (New) The computer system of claim 59, wherein the results of tests to determine the interaction between compounds in the first database and targets in the second database are organized in the third database in terms of whether or not the interaction values fall between specified upper and lower thresholds.

B3

85. (New) The computer system of claim 59, wherein the results of tests to determine the interaction between compounds in the first database and targets in the second database are organized in the third database in terms of profiles of numerical

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

values or meeting specified threshold criteria for specific compounds from the first database with respect to panels of molecular targets in the second database.

86. (New) The computer system of claim 59, wherein the results of tests to determine the interaction between compounds in the first database and targets in the second database are organized in the third database in terms of profiles of numerical values or of meeting specified threshold criteria for specific compounds from the first database with respect to panels of molecular targets in the second database and in formats that allow comparisons to be made (a) between such profiles among subsets of compounds in the first database or (b) between such profiles or groups of profiles of compounds in the first database and a comparable profile of interaction data for a compound or group of compounds not in the first database.

87. (New) The computer system of claim 59, wherein the chemical compounds in the first database are selected from among the compound set comprising LOPAC (List Of Pharmacologically Active Compounds, Sigma/RBI).

88. (New) The computer system of claim 59, wherein the chemical compounds in the first database are selected from among the compound set contained in the U.S. Pharmacopeia Drug Information for the Health Care Professional (USP DI) publication.

89. (New) The computer system of claim 59, wherein records corresponding to the chemical compounds in the first database include at least one of the following:

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

chemical name;

chemical formula;

chemical structure;

molecular weight;

physical chemical properties;

chemical space coordinates;

chemical structural descriptors;

solubility; and

logP..

90. (New) The computer system of claim 59, wherein records corresponding to the chemical compounds in the first database include chemical structural descriptors that are organized in a format amenable to computer-based searching and data analysis methods.

91. (New) The computer system of claim 59, wherein records corresponding to the chemical compounds in the first database are organized by chemical structural relatedness or as chemical descriptor arrays or tables.

92. (New) The computer system of claim 59, wherein records corresponding to the chemical compounds in the first database include chemical structural descriptors that are organized in a format amenable to data analysis using methods of recursive partitioning.

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

93. (New) The computer system of claim 59, wherein records corresponding to the chemical compounds in the first database include chemical structural descriptors that are organized in a format amenable to data analysis using CoMFA software or related methods.

94. (New) The computer system of claim 59, wherein records corresponding to the chemical compounds in the first database include chemical structural descriptors that are organized in a format amenable to data analysis using Catalyst/Hypo software or related methods.

95. (New) The computer system of claim 59, wherein records corresponding to the chemical compounds in the first database include SMILES codes.

96. (New) The computer system of claim 59, wherein records corresponding to the chemical compounds in the first database include 2-D topological descriptors.

97. (New) The computer system of claim 59, wherein records corresponding to the chemical compounds in the first database include 3-D pharmacophore descriptors.

98. (New) The computer system of claim 59, wherein records corresponding to the chemical compounds in the first database include substructure or chemical moiety descriptors.

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

99. (New) The computer system of claim 59, wherein the first database also contains records corresponding to biological information related to effects of the chemical compounds on biological systems.

100. (New) The computer system of claim 99, wherein the records in the first database corresponding to biological information includes information on chemical name, trade names, or alternative compound names and at least one of the following categories:

toxicity;

side effects;

mechanism of action; and

pharmacokinetics.

101. (New) The computer system of claim 100, wherein records in the first database corresponding to biological information related to pharmacokinetic effects of selected chemical compounds on biological systems includes information on at least one of the following categories:

bioavailability;

absorption;

drug distribution;

drug metabolism;

drug excretion;

B3

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

blood-protein binding; and

blood-brain barrier passage.

102. (New) The computer system of claim 100, wherein records in the first database corresponding to biological information related to toxicological effects of selected chemical compounds on biological systems includes information on at least one of the following categories:

teratotoxicity;

mutagenicity;

hepatotoxicity;

renal toxicity;

neurotoxicity; and

cardiotoxicity.

103. (New) The computer system of claim 100, wherein records in the first database corresponding to biological information related to side effects of selected chemical compounds on biological systems includes information on at least one of the following categories:

known receptor interactions;

known enzyme interactions;

behavioral effect;

physiological effect; and

organ effects.

B3

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

104. (New) The computer system of claim 100, wherein records in the first database corresponding to biological information related to mechanism of action of selected chemical compounds on biological systems includes information on at least one of the following categories:

target organ;

major pathway;

minor pathway; and

putative molecular target for mode of action.

105. (New) The computer system of claim 99, wherein records corresponding to biological information related to effects of the chemical compounds on biological systems are organized in a format amenable to computer-based searching and data analysis methods.

106. (New) The computer system of claim 99, wherein records corresponding to biological information related to effects of the chemical compounds on biological systems are encoded using standardized terms or selectable terms from a prepared drop-down menu of possible terms.

B3

107. (New) The computer system of claim 99, wherein records corresponding to biological information related to effects of the chemical compounds on biological

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

systems are encoded using numerical terms such as LD50, ED50, percent absorbed, half-life, and peak concentration.

108. (New) The computer system of claim 59, wherein the targets in the second database are selected from among those comprising the superfamily of G-Protein Coupled Receptors, including the following types and subtypes: dopamine, serotonin, adrenergic, muscarinic/acetylcholine, histamine, adenosine, angiotensin, bradykinin, C5a, chemokine, CCK, endothelin, neuropeptide Y, neurotensin, opioid, somatostatin, tachykinin, vasopressin, galanin, prostanoid, purinoceptors, cannabinoid, platelet-activating factor, thyrotropin releasing factor, leukotriene, corticotropin releasing factor, PACAP, vasoactive intestinal peptide, melatonin, glutamate, and GABA-B.

109. (New) The computer system of claim 59, wherein the molecular targets in the second database comprise receptors that are not G-Protein coupled.

110. (New) The computer system of claim 59, wherein the targets in the second database are selected from among those comprising nuclear receptors or intracellular receptors, including estrogen, glucocorticoid, progesterone, and androgen.

B3

111. (New) The computer system of claim 59, wherein the molecular targets in the second database comprise kinases or phosphatases.

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

112. (New) The computer system of claim 59, wherein the molecular targets in the second database are selected from among those comprising cytochrome P450 enzymes.

113. (New) The computer system of claim 59, wherein the molecular targets in the second database are selected from among those comprising DNA-modifying enzymes or transferases.

114. (New) The computer system of claim 59, wherein the molecular targets in the second database are selected from among those comprising neurotransmitter-related enzymes.

115. (New) The computer system of claim 59, wherein the molecular targets in the second database comprise proteases or carbohydrates.

116. (New) The computer system of claim 69, wherein the molecular targets related to drug discovery and development include nucleic acids.

117. (New) The computer system of claim 69, wherein the molecular targets related to drug discovery and development include carbohydrates.

B3

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

118. (New) The computer system of claim 59, wherein the molecular targets in the second database are selected from among sodium, potassium, calcium, chloride, or ligand-gated channels.

119. (New) The computer system of claim 59, wherein the molecular targets in the second database are selected from among transporters or uptake sites for dopamine, serotonin, norepinephrine, adenosine, glycine, glutamate, and choline.

120. (New) The computer system of claim 59, wherein records corresponding to the molecular targets in the second database include at least one of the following:

molecular target name;

molecular target family, classification or type;

corresponding gene DNA sequence;

amino acid sequence;

3-dimensional conformation or structure;

differential expression across different cell types

location of expression in tissues or cell types;

hydropathy plots; and

biochemical or molecular descriptors.

121. (New) The computer system of claim 59, wherein records corresponding to the molecular targets in the second database are organized in a format amenable to computer-based searching and data analysis methods.

B3

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

122. (New) The computer system of claim 59, wherein records corresponding to the molecular targets in the second database are organized by DNA sequence alignments.

123. (New) The computer system of claim 59, wherein records corresponding to the molecular targets in the second database are organized by DNA sequence homology.

124. (New) The computer system of claim 59, wherein records corresponding to the molecular targets in the second database are organized according to phylogenetic trees.

125. (New) The computer system of claim 59, wherein records corresponding to the molecular targets in the second database are organized by species source of the molecular target used in the test to determine the interaction between chemicals and targets.

126. (New) The computer system of claim 59, wherein records corresponding to the molecular targets in the second database are organized by location of expression in tissues.

B3

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

127. (New) The computer system of claim 59, wherein records corresponding to the molecular targets in the second database are organized by major or minor pathways.

128. (New) The computer system of claim 59, wherein records corresponding to the molecular targets in the second database are organized by distribution of molecular target protein expression across different cell types.

129. (New) The computer system of claim 59, wherein records corresponding to the molecular targets in the second database are organized by distribution of molecular target messenger RNA expression across different cell types.

130. (New) The computer system of claim 59, wherein records corresponding to the molecular targets in the second database are organized by differential expression.

131. (New) The computer system of claim 59, wherein records corresponding to the molecular targets in the second database are organized by differential expression based on different test conditions.

132. (New) A computer system comprising:

a first database containing records corresponding to a plurality of chemical compounds,

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

a second database containing records corresponding to a plurality of molecular targets;

a third database containing records corresponding to the results of tests to determine the interaction between compounds in the first database and targets in the second database, wherein the third database includes records corresponding to the results of tests to determine the interaction between a majority of the compounds selected to comprise a compound set in the first database and a majority of the molecular targets selected to comprise a molecular target set in the second database; and

a user interface allowing a user to view data from the first database, the second database, and the third database as it relates to at least one compound in the first database or as it relates to at least one molecular target in the second database or as it relates to one or more interactions in the third database.

133. (New) A memory for storing data for access by a process being executed by a processor, the memory comprising:

a data structure for maintaining information identifying a plurality of chemical compounds and a plurality of molecular targets, wherein the data structure further maintains a set of information corresponding to results of tests to determine the interaction between the plurality of chemical compounds and the plurality of molecular targets.

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com

134. (New) The memory of claim 134, wherein the chemical compounds are known biologically active chemical compounds.

135. (New) The memory of claim 134, wherein the results are represented in a form that reflects whether each chemical compound binds with a corresponding molecular target.

136. (New) The memory of claim 134, wherein the results are represented in a form that reflects a potency of a binding between each chemical compound and a corresponding molecular target.

137. (New) The memory of claim 134, wherein the data structure maintains a set of information corresponding to results of tests to determine the interaction between all or substantially all of a plurality of compounds selected to comprise a compound set in a chemical compound data structure and all or substantially all of a plurality of molecular targets selected to comprise a molecular target set in a molecular target data structure.

138. (New) The memory of claim 134, wherein the data structure maintains a set of information corresponding to results of tests to determine the interaction between a majority of a plurality of compounds selected to comprise a compound set in a chemical compound data structure and a majority of a plurality of molecular targets selected to comprise a molecular target set in a molecular target data structure.

FINNEGAN
HENDERSON
FARABOW
GARRETT &
DUNNER LLP

1300 I Street, NW
Washington, DC 20005
202.408.4000
Fax 202.408.4400
www.finnegan.com